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Design and simulation of an infrared optical filter suitable for carbon dioxide and CO_2 lasers

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The main objective of this study was to assess the molecular simulation of the design of carbon dioxide (CO_2) and to construct infrared optical filters for the transmission and absorption of the CO_2 laser and the emission of gaseous CO_2 radiation. Semiconductor compounds used to determine the wavelength of infrared transmission and absorption infrared radiation (IR) to produce an IR filter for laser production and gas emission using the Fourier Transform infrared spectrometer (FT-RI) for research purposes. Carbon dioxide molecule simulation has been used based on Hyper 6 simulation programme in potential energy, and kinetic energy, which measures the infrared radiation spectrum. Infrared filters are constructed from the compounds of a semiconductor of Zinc Sulfide supplied (ZnS), Aluminum Oxide (Al_2O_3), Magnesium Oxide (MgO), Lead (II) Sulfide (PbS), and Potassium Chloride (KCl). The data used for evaluation of the optical elements in the IR region based on the transmission and absorption of radiation intensity effective for wavelength detection. The assessment of the detection is indicating transmission and absorption of the wavelengths of CO_2 laser and CO_2 gas molecule under investigation. This study has identified the approach of the result of transmission and absorption of the peak intensities of 10.6, 2.7, 4.3 and 15µm of CO_2 laser and gas radiation emission of the filters in the IR region. The findings of this study have a number of important applications in the IR radiation region.

Keywords: Carbon dioxide, Simulation, Spectroscopy, Infrared filter, CO_2 laser, Semiconductor compound.

1 Introduction

Recently, infrared spectroscopy has developed in a variety of ways for sensitive detection techniques to measure the radiation intestines of a wavelength which emits or absorbs particles or atoms against infrared radiation for analysis. The use of qualitative and measurable analysis of infrared radiation absorbed by organic and inorganic molecules, *i.e.* radiation converted into energy vibrations of molecules[1]. The molecules change their rotational-vibrational motions by infrared radiation by absorbing and emitting energy and change the dipole moment of the molecules, which reflects these symmetrical frequency range molecules[2]. The functional groups and composite characteristic bonds absorbed a wide range of infrared wavelength radiation that form the infrared spectrum for the study of atoms. Semiconductor materials and compounds are transparent to infrared radiation and block the visible range of light irradiation[3].

Carbon dioxide is the largest anthropogenic gas that contributes to climate change in the Earth's atmosphere and causes ambient air to heat up. A gaseous CO_2 is an established carbon cycle of plant life that the molecule has been the object of interest from several scientists in recent decades[4]. Carbon dioxide is the vibration mode of the linear molecule and implies in the dipole moment of the molecule that CO_2 emits a large range of infrared radiation. The energies of infrared radiation are inversely proportional to the wavelength or directly proportional to the number-waves[5].

CO_2 laser is a powerful device used in a wide range of applications such as industrial and medical applications[3]. CO_2 molecular gas lasers emit in the infrared range due to atomic transitions between rotation and vibration states. The most popular laser in the infrared range is the CO_2 laser, which emits radiation in the range of 8 to 18 µm, but the most useful wavelength center is 10.6 µm[6].

The most important issues to deal with infrared radiation are filtering and detection tools and processes. Source radiation absorbed by the atoms of the material used, which usually occurs as very narrow lines of characteristic wavelength from the infrared to far infrared range of the spectrum[7].

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Many semi-conductor materials were cloudy with visible light and relatively transparent at infrared radiation. This is due to the influence of the semiconductor compound on band-to-band absorption into visible radiation[8]. In infrared radiation, absorption is mainly caused by the absorption of free carriers and transitions to impurity levels. A carbon dioxide molecule may not absorb radiation unless the incoming infrared radiation is of the same frequency as one of the basic modes of vibration of the molecule. This means that the vibrationalmovement of small parts of the molecule increases while the rest of the molecule is left unaffected[9]. The fundamental vibrations of the CO_2 molecule are asymmetric stretches giving a sharp band in the IR at 2350 cm^{-1}, while the two similar scissoring or bendingvibrations and, therefore, have the same frequency as what appears in a 666 cm^{-1} IR spectrum[10, 11]. The photon with the infrared spectrum excites the vibrations of the molecules and causes the heat to occur at a certain level due to the movement of the atom far or toward one another. The energy of the molecules and the frequency only the permitted energy of the photons will excite atoms to vibrate due to absorption in this level. However, the CO_2 measurement technique used two methods of concentration measurement using the infrared absorption principle, energy, wavelength, temperature and infrared radiation emitted from the properties of CO_2 molecules[12].

Infrared optical filters have been required for a wide range of laser electro-optical applications. However, the exact degree of attenuation and reflection or polarization required filter characteristics to precisely monitor the filter function for frequency[13]. Infrared filters are categorized into four categories based on their application.Filters are possible to be passed infrared radiation and blocking other wavelengths or block infrared (only). Infrared cutoff filters designed for blocking or transmitting infrared wavelengths, but passing visible light[14].

The main theory of the Hyper 6 simulation program is the concept of a potential energy surface and the distinction between classic and quantum energy, kinetic and potential energy. Density functional theory was the dominant method for quantum mechanical simulation of the linear molecule of carbon dioxide optics. This programme offers an approach to the problem of defining a potential energy surface for the movement of CO_2 and the infrared spectrum of molecules and the transmission of defined and characteristic peak in the infrared region.

2 Experimental & Methods

Samples of semiconductor compounds of various sizes which measured their spectra in the IR region of each compound with a FT-IR spectrometer for each compound of interest[15]. The samples were adapted for measurement by grinding them with potassium bromide powder and pressing to form a disc. The powdered compounds are mixed using different concentrations in disc pellets with a series of thin, thick samples.

A common approach of preparing solid samples for IR analysis was the pellet technique. The principle here is to grind the particles below the wavelength of the incident radiation, which will pass through the thickness of the sample limited scatter. The solid sample is crushed into a fine powder with a hand grinder and a quantity of KBr used for this method has been soft salts. The powder compounds use to prepare pellets in the shape of a round disc of different thickness to usually yield adequate results.

Potassium bromide (KBr) is widely used as infrared optical windows that are high transmitted from ultraviolet to infrared radiation in the range of (0.25 - 25 μm)[16]. Compounds of semiconductors of Zinc Sulfide (ZnS), Aluminum Oxide (Al_2O_3) Magnesium Oxide (MgO), Lead (II) Sulfide (PbS) and Potassium Chloride (KCl) uses in different weight in groups such as Pbs, MgO and ZnS, and Al_2O_3 addition to KCL and as MgO and Al_2O_3 all mix with Potassium bromide KBr. The salt sample is put in a cylindrical holder and pressed together into a pellet shape suitable for measurement[17].

Spectroscopic analysis carried out is using spectrometer FT-IR to acquire the relation between the wave-number and absorption or transmission of the intensity of the material semiconductor compound in the IR region. The samples were mixed with different weight and the amount of potassium bromide with two or three of the compounds of different weight and different ratios. The samples powder as places in the disc diameter of 2.5 cm and then compressed to a manual pressure up to 15 tons and after the samples have become the tablets placed in the FT-IR spectrometer for data collection. The FT-IR-8400S uses to measure the samples of the mixed semiconductor compound of different weight with a maximum resolution of 0.85 cm^{-1}, and achieves the best signal-to-noise ratio in the range of 20,000:1 or better (peak-to-peak, 04 cm^{-1} resolution averaged over 1minute). Data of semiconductor compounds using an FT-IR spectrometer of different samples to collect IR irradiation transmission and absorption of recording spectra.

3 Results and Discussion

The IR spectra measurement has displayed the absorption and transmission of the infrared radiation percentages against wave-numbers indicating the desired wavelengths under the study. Infrared spectra of CO_2 laser and CO_2 gas and wavelengths under investigation for monitoring the transmission and absorption of the intensity are appearing from the different compounds[18]. New approaches, techniques for wavelength depend on semiconductor different compound properties.

The resulting of the simulation and measurement of the CO_2 molecule structure is designed with the Hyper 6 program. Therefore, the CO_2 assessment of infrared indicates the optical properties of Molecule absorption and transition in the region. The result of the program simulation shows the infrared spectrum of the CO_2 molecule shown in the Fig. 1 and the molecule diagram. The spectrum of the molecule in the figure shows the two waves-numbers of 2479 cm^{-1} and 629 cm^{-1}that represent an asymmetrical stretch and scissoring of the molecule.

Spectrum of sampling of mixed compounds (A). (PbS+ MgO+ ZnS+ KBr) represents a transmission peak in the wave-number range (2310.56 – 3697.29) cm^{-1} as showing in Fig. 2.

Figure 2 shows the peak intensity of 11.5% transmission of IR in 2310.56 cm^{-1} that typically in the wavelength 4.327μm, which is under investigation. In addition, the peak transmission of 8% 3697.29 cm^{-1} normally in the wavelength 2.704 μm covers the first wavelength under investigation. Spectrum of samples of different weight and ratios of (B). (PbS + MgO + ZnS + KBr) represented a transmission peak in wave-number 2295.13 cm^{-1} as showing in Fig. 3.

Figure 3 displays the peak radiation intensity of 2.85% transmission of IR the 2295.13 cm^{-1} wave-number in the wavelength of 4.357 μm that covers the second wavelength of the CO_2 molecule. Sample

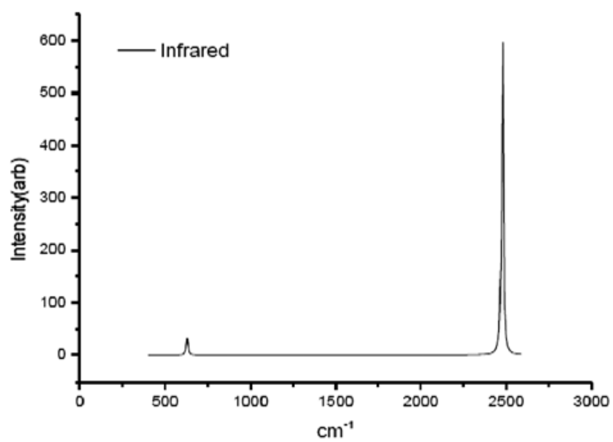

Fig. 1 — Infrared spectrum of vibrational modes of CO_2

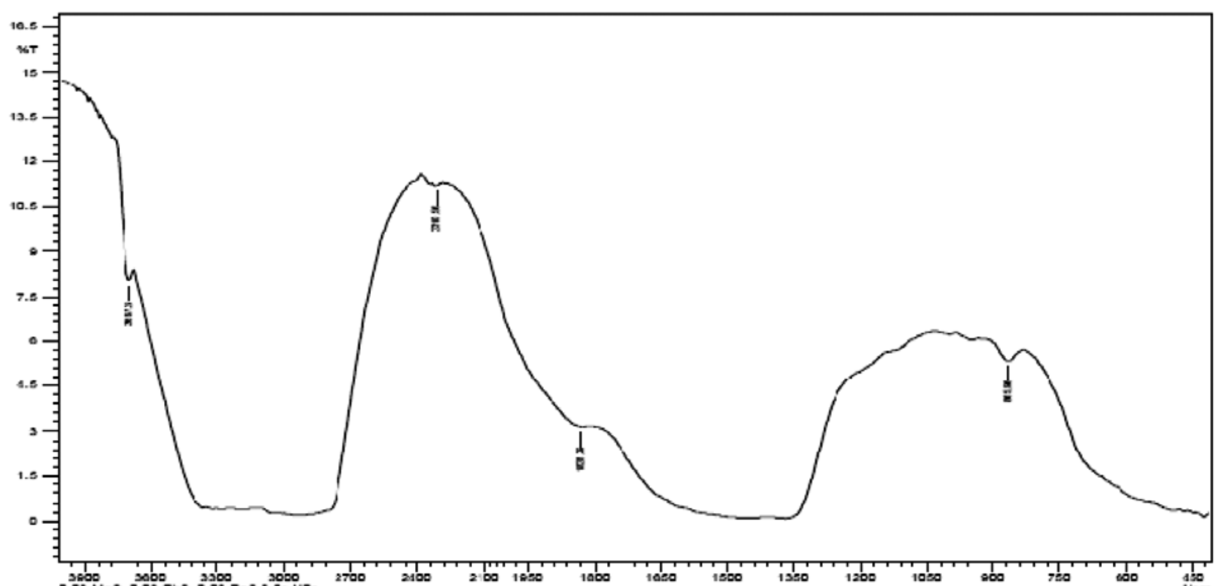

Fig. 2 — shows the FTIR spectrum of sample A,(PbS+ MgO+ ZnS+ KBr)

compounds (C) of different weight and ratio (PbS+ MgO+ ZnS+ KBr) represented a transmission peak in wave-number 3662.57 and 940 cm^{-1}as shown in Fig. 4. The IR intensity of 15% transmission of the 3662.57 cm^{-1} in Fig. 4 typically in the wavelength 2.730 µm it covers the first wavelength studies and 65% transmission of 10.6 µm. Spectrum of samples of different weight and ratio (D), (PbS+ MgO+ ZnS+ KBr) represented a transmission peak in the wave-number range (2347.21 – 3703.07) cm^{-1} which displayed in Fig. 5. Figure 5 shows the peak intensity of 95% transmissions of IR in 2347.21 cm^{-1} normally in the wavelength 4.260µm as the second wavelength study. In addition, the transmission of 8% of the 3703.07 cm^{-1} is in the wavelength of 2.700µm, which covers the first wavelength under analysis. A spectrum of the sample (E) of ($KCl+Al_2O_3+KBr$) represents no transmission shows that in Fig. 6.

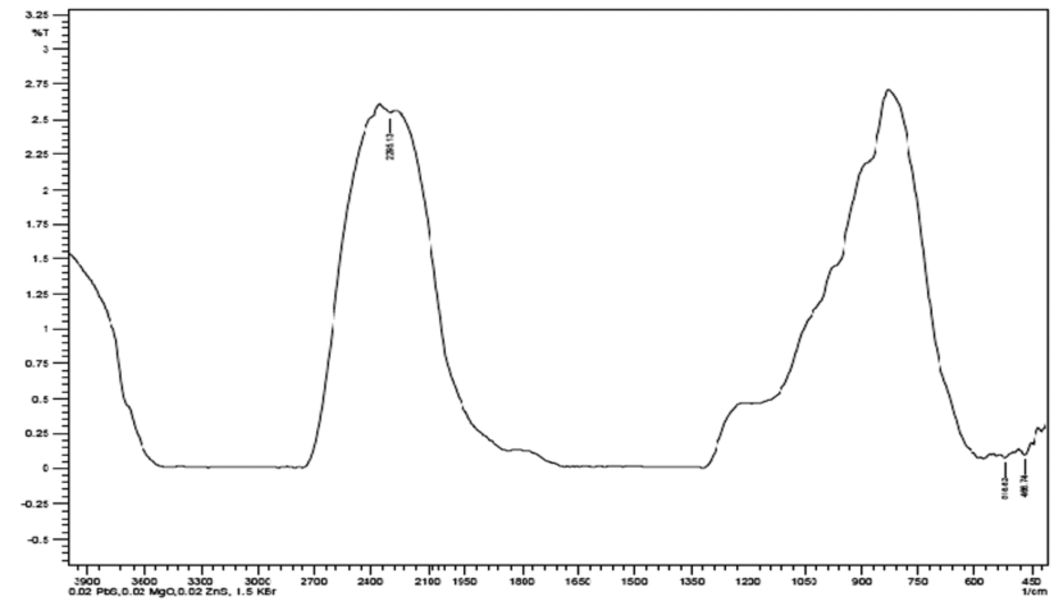

Fig. 3 — shows the FTIR spectrum of sample B,(PbS + MgO + ZnS + KBr)

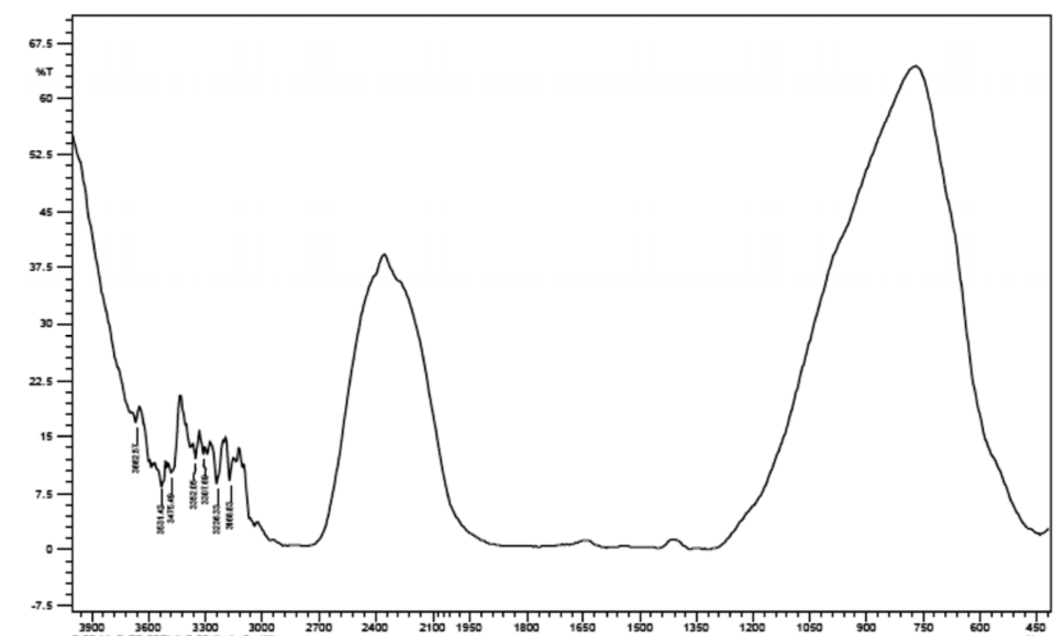

Fig. 4 — shows the FT-IR spectrum of sample C,(PbS+ MgO+ ZnS+ KBr)

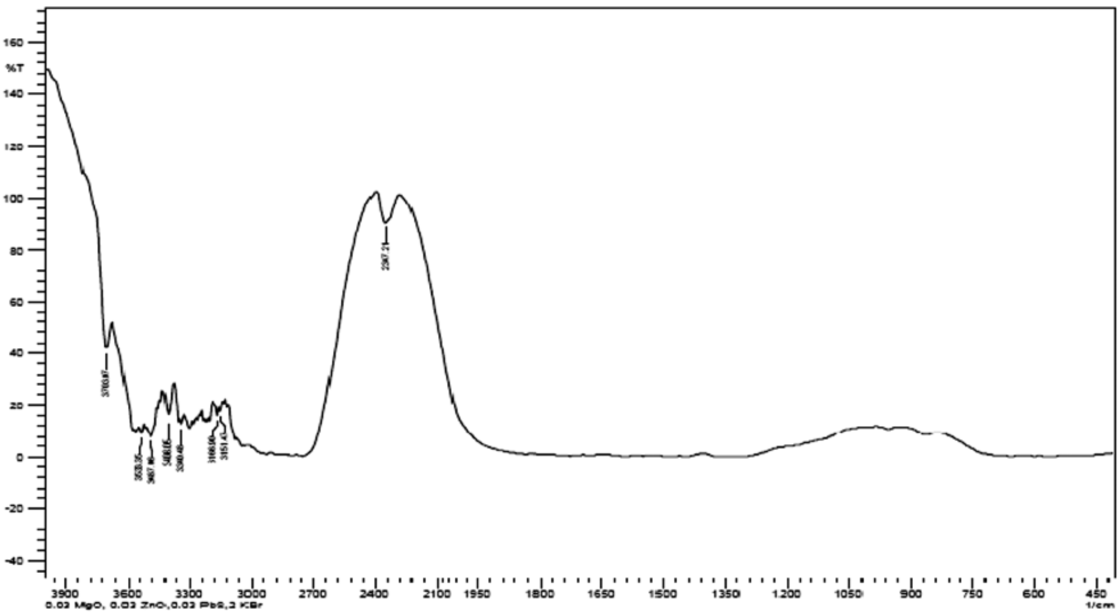

Fig. 5 — shows the FTIR spectrum of sample D, (PbS+ MgO+ ZnS+ KBr)

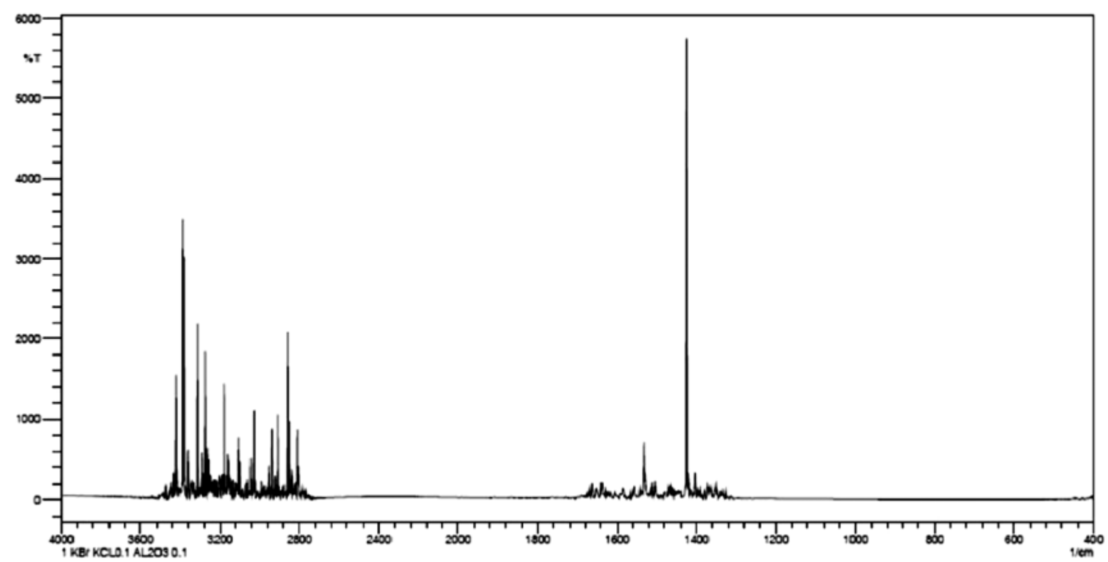

Fig. 6 — shows the FTIR spectrum of sample E, ($KCl+Al_2O_3+KBr$)

Figure 6 shows the IR intensity of 0% transmission of the wavelengths is blocked with the filter. A spectrum of the composite sample F ($MgO + Al_2O_3+ KBr$) doesn't show any wavelength transmission of the CO_2 gas and CO_2 laser as shownin Fig. 7.

Figure 7 The IR intensity of 0% transmission of the range wavelengths under investigation. Spectrum of sample (H) that made for (PbS + MgO + ZnS + KBr) represented a transmission peak in the wave-number range (2325.58 – 3703.07) cm^{-1} shows that Fig. 8. The infrared radiation in Fig. 8 indicates that the transmit intensity of 0% of the study range of the wavelength range is blocked.

4 Discussion

The detection of semiconductor compounds displays spectrum of IR transmission of 10.6, 15, 4.3 and 2.7μm wavelength that is characteristic of the wave-numbers of 940, 2325.58, 666.67 and 3703.70 cm^{-1} respectively for CO_2 infrared radiation and CO_2 laser[19]. However. The simulated spectrum of CO_2 the molecule is compared to the difference of the

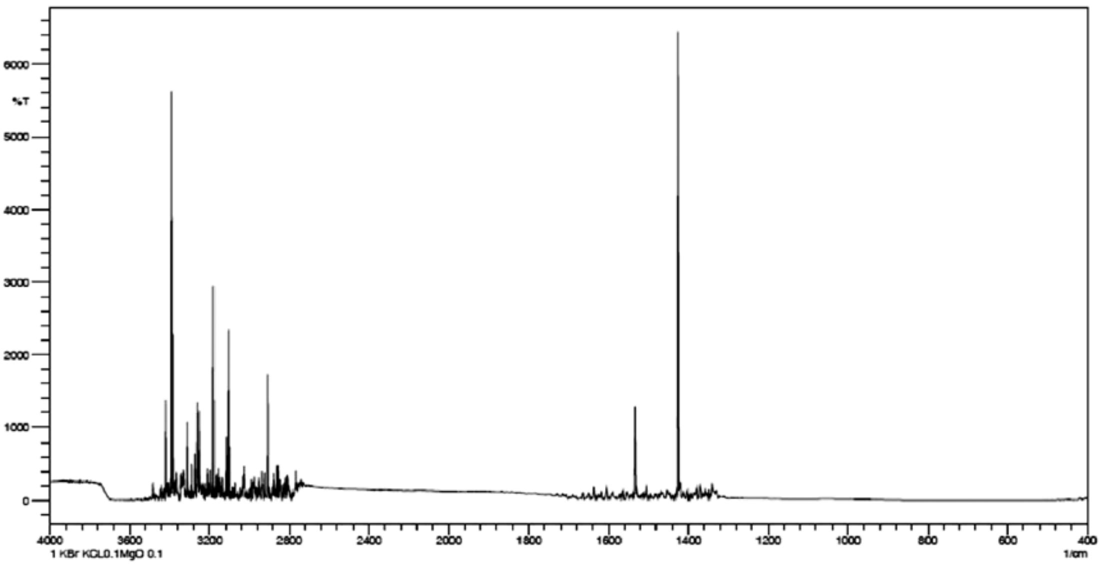

Fig. 7 — shows the FT-IR spectrum of sample F,($MgO + Al_2O_3$+ KBr)

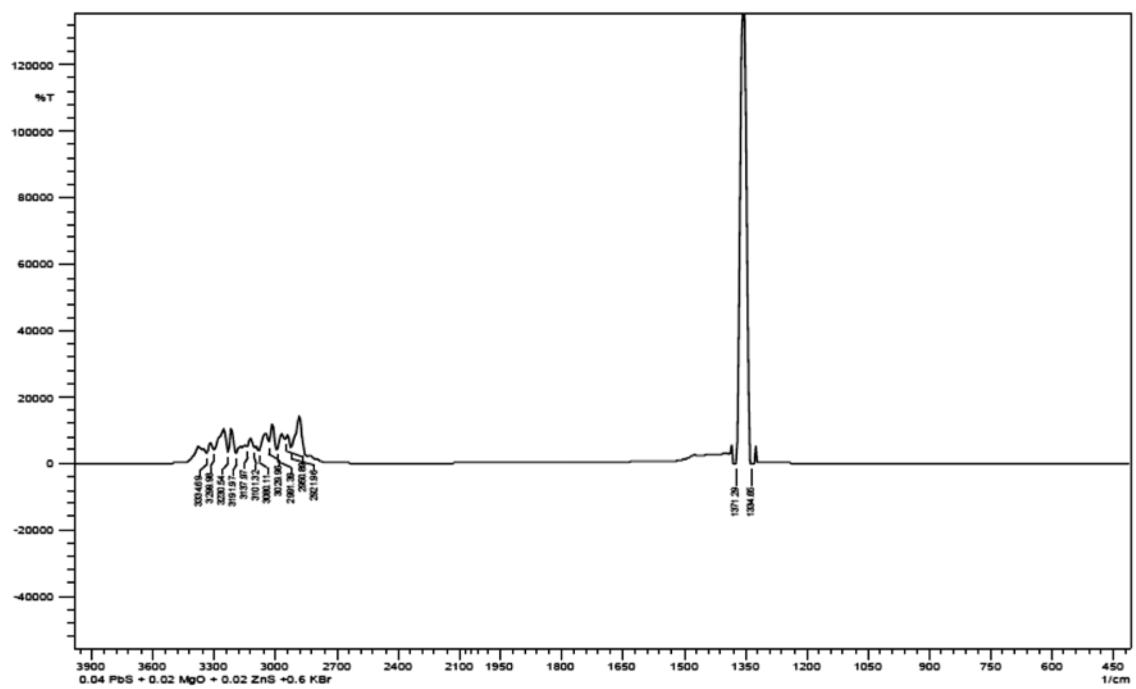

Fig. 8 — shows the FT-IR spectrum of sample H, (PbS + MgO + ZnS + KBr)

literature values in the range of 5.47% to 5.57% of the peak spectrum and the filter transmission region usually in the range.The infrared radiation from the source which is absorbed by atoms of semiconductor compound used is mainly in the form of very narrow lines of characteristic wavelength originating from near infrared to far infrared range of spectra[19].

When only the peak in the spectrum reflects the intensity of infrared radiation transmitted through the filter. This may include some means of identifying the percentage of the transmission[20].

The spectra in the above figures in groups A, B, C, and D show the radiation transmission of the wavelength, that the filter path different peak intensity due to the mixed compound concentration and the thickness of the samples.Group E, F, and H displayed in the figures the absorption of the wavelength of CO_2 radiation at 2.7, 4.3, 10.6 and 15 μm. While the compounds of the group E, F and H present a lower background for IR radiation without transmission or absorption for the wavelength understudies. The current detection of absorption and transmission revealed that optical elements of the infrared radiation region can be used for various wavelength identification applications. So that optical filters are possible to be fabricated from these compounds for the desired wavelength in IR for the CO_2 gas emission and CO_2 laser wavelengths mentioned above in addition, the control of the filter thickness, the radiation transmission intensities percentage can be controlled.

5 Conclusions

The purpose of this study is studying the transmission and absorption of the peak intensities of 10.6, 2.7, 4.3, and 15 μm of CO_2 laser and gas emission in the IR region. The results of the simulation provided a spectrum of CO_2 data consistent with published values in the literature and in the design of their filters. The spectrum is typically within the range requested for the transmission and blocked region.

The simulation results provided a spectrum of CO2 data that agreed with literature values and for the filter, the design is typically in the range request for transmission and block regions. The results of this show that semiconductor compounds in A, B, and C groups used possibly the wavelengths required. The compounds of semiconductors groups E, F, and H in the study did not allow the transmission and absorption of the study wavelengths due to the high background IR for the selected wavelengths. The current data of semiconductor highlight the importance of this material as an optical element in the IR wavelength for several applications in IR technology.

This study has demonstrated that the wavelengths and intensities of radiation blocks and decrease through IR filters, which produces with this material for laser. While for CO_2 gas emission absorbed or used as a filter vision in CO_2 gas cloud in the fired fuel system or firing accidentally. The findings of this study have a number of important applications for the future used in the IR radiation region.

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